

Recent Basic Energy Sciences (BES) Accomplishments

Presented below are some significant BES program accomplishments from FY 1999, FY 1998, and FY 1997. These vignettes appear in the BES portion of the President's FY 2001, FY 2000, and FY 1999 Budget Requests to Congress, respectively. The selected program highlights are representative of the broad range of studies supported in the BES program. These brief accounts describe the discovery of new knowledge, the rapidity with which such new knowledge can often be incorporated into other scientific disciplines and into the commercial sector, and the great potential of new knowledge for future impacts in energy production and use.

Selected FY 1999 Scientific Highlights/Accomplishments

Serendipitous Applications of Research in the Physical Sciences to the Life Sciences. It has long been recognized that tools and concepts developed in the physical sciences can revolutionize the life sciences. One need only consider the impact of x-ray synchrotron radiation and MAD (multiple wavelength anomalous diffraction) phasing on macromolecular crystallography; both were developed within the BES program. In FY 1999, many of the annual BES program highlights illustrate the rapidity with which advances in the physical sciences are impacting the life sciences. Two examples are given here. First, new techniques of nuclear magnetic resonance (NMR) are being used to study the molecular structures of solid protein deposits implicated in brain diseases such as Alzheimer's Disease and BSE (Mad Cow Disease); both diseases involve the transformation of normal, soluble proteins in the brain (whose structure is known) into fibers of insoluble plaque (whose structure is largely unknown). Second, a nano-laser device has been shown to have the potential to quickly identify a cell population that has begun the rapid protein synthesis and mitosis characteristic of cancerous cell proliferation. Pathologists currently rely on microscopic examination of cell morphology using century-old staining methods that are labor-intensive, time-consuming, and frequently in error.

Materials Sciences Subprogram

Seashell Provides Key to Strong Composites. Mollusk shells have evolved over millions of years to provide hard, strong, tough shelters for fragile occupants. These outstanding mechanical properties derive from a laminated construction of alternating layers of biopolymer – a biologically produced rubber – and calcium carbonate, commonly known as chalk. It has been recognized for decades that materials with alternating hard and soft layers absorb energy and impede cracking. Unfortunately, it has proven difficult to transcribe seashell-like designs into manufacturable materials. Now, a rapid, efficient self-assembly process has been developed for making “nanocomposite” materials that mimic the construction of seashells. This process can be generalized and should lead to materials with unprecedented mechanical properties.

Imaging Fluid Distribution and Flow in Materials. Dramatic pictures of the distribution and flow of fluids inside intact objects and porous solid materials have been obtained by magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR). The ability to observe such images and spectra results from the use of noble gases, particularly xenon, magnetically polarized by means of a laser. This advance makes possible the observation of MRI pictures and NMR spectra in ultralow magnetic fields. The technique produces brilliant pictures (up to a millionfold increase in brightness) and provides a new capability for noninvasive investigation of flow and transport. The images and spectra allow the characterization of atomic distribution and flow from the smallest scale of nanotubes to the largest scale of macroscopic samples. The flow of fluids through solid materials is a crucial component of many industrial processes from the catalytic conversion of petroleum to the containment of toxic environmental agents. These advances will eliminate the need for high magnetic fields in some applications of MRI and NMR, a welcomed event given the cost, bulk, hazard, and lack of portability of the magnets used in contemporary instrumentation.

New Fullerene Species Synthesized - Stickyball, C₃₆. A new fullerene species, C₃₆, has been synthesized and produced in bulk quantities for the first time. Fullerenes or “buckyballs” are hollow clusters of carbon

atoms. They have been studied extensively since the Nobel prize-winning discovery of C_{60} in 1985 (supported by BES). C_{36} is the smallest fullerene discovered to date and is characterized by unusual and potentially very useful properties. For example, in contrast to C_{60} molecules, which interact only very weakly with one another, C_{36} molecules stick together – hence the nickname "stickyballs." The lower fullerenes, such as C_{36} are predicted to have more highly strained carbon bonds, resulting in exciting properties for those molecules such as very high chemical reactivity and high temperature superconductivity. The synthesis of C_{36} is particularly significant, because previously it was believed that any fullerene smaller than C_{60} would be too unstable to isolate in bulk.

Seeing Clearly Now. Using a new imaging technique called Z-contrast imaging, researchers have achieved the highest resolution electron microscope image of a crystal structure ever recorded, resolving adjacent columns of silicon atoms separated by a scant 0.78 angstroms (3 billionths of an inch). Better resolution enables scientists to see and understand important details they had not been able to see before. This technique also offers both high spatial resolution and the ability to distinguish different kinds of atoms. The precise atomic-scale structure of a material controls the performance of materials for semiconductor devices, superconductors, and a host of other applications. Combined with improved electron imaging optics currently under development, this result promises to revolutionize the atomic-scale understanding of materials.

New Family of Bulk Ferromagnetic Metallic Glasses for Energy Efficient Motors and Transformers.

New rules for designing alloys have been developed that enable the creation of a family of bulk metallic glass alloys. These alloys exhibit outstanding ferromagnetic behavior with virtually no energy loss. These new alloys are at least 65 percent iron plus contain up to seven other elements. Until now, such alloys could only be produced as thin foils. Commercial transformers based on the thin foil ferromagnetic metallic glasses are in service, but their size and application are limited due to difficulties in thin foil assembly and manufacturing processes. The new bulk glasses can be cast into exact shapes and substituted into the standard assembly processes now in use for traditional crystalline materials. It is expected that the availability of bulk ferromagnetic glasses will decrease the energy losses of transformers by about 2/3 compared to today's transformers made from crystalline ferromagnetic materials. That's good news for electric utility customers, since it is estimated that power-distribution transformer losses cost about \$4 billion annually.

Universal Magnetic Behavior in High-Temperature Superconductors. Understanding high temperature superconductors remains one of the most significant research issues in condensed matter physics. The observed properties of two major classes of high temperature superconductors initially appeared to be significantly different from one other, leading scientists to believe that the fundamental interactions responsible for the superconducting behavior were quite different in the two materials. However, recent neutron scattering results have shown that the superconducting behavior of both major classes of superconductors is connected to excitations of the magnetic spin system in each material. The new results offer insight on high-temperature superconductivity including the promise that a single physical mechanism can account for this phenomenon.

Chemical Sciences Subprogram

Measuring Chemical Processes in Combustion One Molecule at a Time. A powerful new experimental instrument just completed at the Combustion Research Facility promises to provide new information about how molecules dissociate when given enough internal energy. Understanding such processes is critically important for combustion, because, at the high temperatures of combustion, dissociation occurs in a variety of ways that are difficult to observe, model, and predict. In the experiment, pulses of laser light a few femtoseconds in duration pump enough energy into a molecule to cause it to dissociate. (One femtosecond is one millionth of a billionth of a second.) A second femtosecond laser pulse ionizes the molecular fragment during the dissociation process. From the simultaneous measurements of the fragments produced by the second laser, the details of the dissociation process can be extracted. These measurements are made one molecule at a time. This new experimental facility promises to be a tool of unrivaled power for the validation of predictive models and theories of chemical reactions.

New Designs for Molecular Wires Help Mimic Photosynthesis. One way to capture and store the sun's energy is to design systems that mimic photosynthesis. In nature, biological systems use charge separation to store energy. This charge separation occurs by transfer of an electron from a photoexcited donor molecule through a bridge molecule to an acceptor molecule. Researchers have recently constructed donor-bridge-acceptor systems in which the bridge – or molecular wire – is a conjugated organic molecule analogous to natural carotenes that transfer charge over long distances. This research may lead to new molecular devices for efficient charge separation and storage.

New Insights into Surface Catalysis. One of the oldest problems in surface-catalyzed reactions is understanding how the molecules actually come together on a metal surface. Researchers studying the hydrogenation of acetylene on crystalline nickel using sophisticated atomic and molecular beam preparations and subsequent thermal desorption spectroscopy demonstrated that this simple reaction proceeds via hydrogen absorbed into the bulk of the metal rather than adsorbed on its surface, as previously thought. This startling discovery has changed the way we think about industrial hydrogenation catalysts such as Raney nickel and palladium, and may have general implications for heterogeneous catalysts presently used in energy-intensive industries such as ammonia production (the Haber Process).

First Observation of Relativistic Thomson Scattering – 60 Years After its Prediction. British physicist J. J. Thomson, who identified the electron in 1897, showed in 1906 that light could cause electrons to oscillate up and down and reemit at the same frequency in a dipole pattern; this phenomenon was subsequently termed Thomson scattering. Nearly a century later, researchers have demonstrated a new phenomena – relativistic Thomson scattering – in which electrons oscillate in a more complex figure-8 pattern and emit light at both the exciting laser frequency and multiples of that frequency, each emitted in a different direction. The more complex pattern results from the electron interacting simultaneously with both the electric and magnetic fields of the laser light. To observe this phenomena, the research team built a tabletop neodymium-glass laser and compressed its billionth-of-a-second pulses by a factor of about 1,000, boosting their power to 4 trillion watts of very high-quality beam. This experiment is an important milestone in the study of nonlinear optics with electrons unbound to atoms. Furthermore, this work may lead to new laboratory tabletop x-ray sources producing very short x-ray pulses useful, for example, for probing molecular motion during reactions.

Engineering and Geosciences Subprogram

Making Waves. Unfortunately, many facets of nature exhibit chaotic changes, driven by external forces, never settling down to a predictable state. Progress has been made in understanding one kind of chaos in which information travels from one point to another by means of traveling waves. Examples include the ripples on a wind-blown lake, light in a laser, weather patterns, and even the fibrillation of a human heart. In order to understand this kind of chaos, scientists studied the flow patterns in a thin layer of fluid heated from below. In certain fluid mixtures, the patterns move laterally like waves on a pond. The key discovery is that these patterns can be understood in terms of so-called phase defects, which are places where the waves circle around a point in a pinwheel-like motion. Looking at only the defects to understand the entire pattern is much like keeping track of traffic jams and accidents to understand the operation of a freeway system. The next step will be to predict how the patterns change with time. If present ideas are confirmed, they could be useful controlling such important phenomena as heart fibrillation, and controlling lasers used in communications, cutting and welding.

Changes in Seismic Properties of Rocks Detects Damage. Seismology uses the reflection and transmission of elastic waves to locate subsurface features of interest. Various types of rocks respond differently to different kinds and frequencies of waves. The theoretical geophysics program has developed new techniques to study these phenomena. The research examines rock behavior through ultrasonic resonance experiments, which show that rock has both a rapid resonance response and a slow resonance response. The resonance between the vibrational modes gives the rock a memory of the shaking it has been through. The resonance behavior has implications for accurately locating subsurface features, and for understanding strong ground motion damage patterns during earthquakes when the resonant modes of regions of different ground properties couple with those of man-made structures. A similar resonance response is also characteristic of damaged man-made materials such as metals, ceramics and composites.

Thus the nonlinear elastic wave studies can contribute to understanding and testing the characteristics of most man-made materials as well as rock or concrete.

Energy Biosciences Subprogram

Orienting Molecular Syntheses. A component of plant cell walls that severely restricts the use of the carbohydrates in plant biomass is lignin. Lignins are aromatic polymers that make up a significant fraction of the earth's renewable carbon resources. Research has provided evidence that the biosynthesis of these large polymers from smaller lignol units does not proceed in a random fashion, as was previously thought. Novel plant genes have been discovered that encode proteins that serve as a scaffold, helping to hold the lignol units in the right orientation as they are joined together by other biosynthetic enzymes. These results have broad implications for the efficient use of plant biomass as well as offering new strategies for enzyme catalysis in an industrial setting.

Plant Cell Walls. The characteristics of plant cell walls – the major energy component of renewable biological resources – vary to meet the structural, metabolic, and developmental needs of different plant cell types. The biosynthesis of the plant cell wall is precisely regulated to conform to these constraints; however, relatively little is known about how such variation is achieved during cell wall formation. Researchers recently identified an enzyme responsible for modifying the xyloglucan polymer backbone, an important factor in determining cell wall strength. This discovery offers the potential to isolate similar enzymes that modify cell wall properties. A better understanding of plant cell wall biosynthesis can eventually improve the properties of wood and other biomass materials through the efficient design of specific complex carbohydrates and other renewable carbon resources.

Designer Enzymes. Research on fatty acid desaturases and hydroxylases has deciphered the mechanism that controls how these two types of enzymes introduce a double bond (desaturase) or a hydroxyl group (hydroxylase) at specific sites along the carbon atom backbone of long-chain fatty acids. This knowledge of the active site of the two enzymes has enabled the modification of the gene that encodes the desaturase for a specific fatty acid to change it into the hydroxylase and vice versa. Both enzymes perform important tasks in altering the melting response of the fatty acid to heat. This pioneering work lays the groundwork for future advances in designing vegetable oils—which have hundreds of potential uses from heart-healthy margarine to lubricants and nylon.

Selected FY 1998 Scientific Highlights/Accomplishments

Materials Sciences Subprogram

Helping to Solve the Mystery of High-Temperature Superconductivity. Understanding high-temperature superconductivity, discovered in 1987, remains the outstanding problem in modern condensed matter physics. Recent neutron scattering experiments suggest that the electric current in high temperature superconductors may be like “stripes” of flowing current separated by stripes where current does not flow. These stripes can be static or dynamic (like the stripes on our flags, waving in the wind). These and other experiments point to a very different electron pairing mechanism than that seen in low-temperature superconductors. Once the pairing mechanism is understood, it will be easier to find materials with higher critical superconducting temperatures and better mechanical properties.

Magnetic Resonance Imaging (MRI) Without Magnets. Striking, high resolution MRI images have been obtained without the need for high field magnets or high frequency detectors normally required for MRI. The breakthrough involves MRI enhancement by noble gases magnetically polarized (100,000 fold) through laser treatment. A new ultra-low-field MRI instrument now makes it possible to obtain extremely bright MRI pictures of polarized samples in the earth's natural magnetic field, which is thousands of times weaker than fields obtained from traditional MRI magnets (which are bulky, expensive, and often hazardous). The new instrument has been used with localized injection of polarized xenon solutions into human blood to provide the first observations of the real-time process of xenon penetrating red blood cells. (Xenon is an inert gas and an FDA-approved anaesthetic.) This combination of techniques opens the way to provide high resolution MRI images of localized areas in animal and human subjects.

Discovery of New Materials Using LEGO. Of the enormous number of combinations of elements in the periodic table, only a very small fraction are used in real materials. It is quite certain that materials with optimum properties for various applications have not yet been discovered. For example, high-temperature superconductivity occurs in ceramic compounds with a most unlikely combination of elements. A new strategy using fast computers and concepts from quantum mechanics has been developed to search for "winning combinations" of atoms to produce materials with improved physical properties. This approach -- Linear Expansion in Geometric Objects (LEGO) -- recognizes that even complex crystal structures can be viewed as a collection of simple geometric objects such as dumbbells, triangles, etc. By assigning each geometric object an energy value, computers can rapidly scan hundreds of thousands of candidates looking for the lowest overall energy and, therefore, the most stable structures. LEGO has already predicted several new intermetallic compounds missed through conventional approaches.

Electrically Conducting Nanoscale Ropes. Incredibly light synthetic metals with a potential electrical conductivity 50-100 times better than copper per weight are being made from carbon nanotubes doped with metals. First discovered in 1991, nanotubes are a new class of materials formed from graphite-like sheets of carbon rolled into exquisitely small cylinders. They self organize in the vapor phase during growth to form well ordered crystalline bundles of individual nanotubes. The introduction of dopant atoms, such as potassium or lithium, into the open spaces between adjacent tubes within a rope can increase electrical conductivity significantly at room temperature. Doped nanotube ropes are also attracting increased interest as constituents of novel nanoscale device structures and as replacements for pure lithium metal in Li ion batteries.

Molecular Bricks for Nanotechnology. Lightweight materials are commonly composed of polymers, which are long chains of atoms. The chains are difficult to order completely, which limits their functionality and durability. Researchers have recently demonstrated new possibilities for the design of polymers using nano-objects, which can be regarded as molecular bricks. These bricks, which might have shapes as diverse as those of nature's proteins, create a toolbox for the design of lightweight materials that could self assemble into structures with surprising functionality. Using the first elements of this toolbox, a spherical nanostructure has been created that has internally continuous channels; some channels transport water and ions, while others block water but accept organic substances. These nano-sponges could trap toxic metals from water streams.

What Makes Stainless Steel Stainless? Corrosion damage is estimated to cost the U.S. 4.2 percent of the Gross National Product each year. Metals can be used in industrial and technological applications only when appropriately protected. In the case of stainless steel and many other metals, protection is provided by a thin oxide film that prevents further corrosion. However, the structure of these oxide films has remained a mystery despite decades of study. Recent research using surface-sensitive synchrotron x-ray diffraction with a combination of electrochemical experiments has now unambiguously determined that the oxide film on pure iron has a very fine-grained, nanocrystalline structure. Results for iron-chromium alloys (e.g., stainless steel) have shown that the oxide films are also nanocrystalline. This overturns the long accepted belief that stainless steel is corrosion resistant because its oxide film is non-crystalline. These surprising results provide a more realistic basis for understanding corrosion resistance and for the development of better corrosion protection coatings.

Do Cracks "Melt" Their Way through Solids? Predicting and explaining why, how, and when solids fracture is a significant scientific challenge. The driving force for fracture is intensification of the local stress at a crack tip, yet the mechanism by which local strain is dissipated during crack propagation is not well understood. Can strain energy be dissipated via "local melting" around the crack tip? Recent computer simulations of crack formation predict this intriguing possibility. Simulations indicated that the melting in front of a crack tip can lead to catastrophic fracture. Using high-voltage electron microscopy, observations of moving crack tips in an intermetallic compound confirmed the prediction of the computer simulations and showed the development of melted and rapidly re-solidified regions adjacent to the crack tip. This new picture of fracture as a stress-induced melting process may lead to new approaches to stress-corrosion cracking in the automotive, aerospace, power generation, and ship building industries.

Smart Filters. New materials with tailored pore sizes and pore chemistry can selectively remove deadly heavy metals -- such as mercury, lead, and silver -- from water. Researchers discovered that precise control over the amount of water in the pores of porous silica enabled the insertion of useful organic molecules on the walls of the pores. Using this knowledge, monolayers of organic sulfur compounds were bound to the internal surfaces of porous silica to prepare selective filter materials. The high surface area of the porous silica (a few grams have as much surface area as a football field) coupled with the bonding characteristics of the organic compounds results in high filtering capacity and high selectivity for specific contaminants. In addition, pore openings in the silica are designed to be too small for microbes to enter and digest the contaminants, later causing human illness from, for example, mercury contamination. The filter materials can purify highly contaminated water in a single treatment to a level that exceeds drinking water standards. The filters can also be recovered and reused after removing the contaminants.

A Line in the Sand. Granular materials like gravel, salt, or dry chemicals are ubiquitous in our daily lives and central to many industrial processes, yet controlling their motion is both surprisingly difficult and not well understood. For example, granular material subjected to a driving force remains at rest until a minimum "critical force" is applied; then it moves in uncontrollable events like avalanches. Inefficiency in handling granular materials may result in the loss of up to 40 percent of the design capacity of industrial plants. In its retrospective of the last 50 years, *Physics Today* highlighted the emerging science of granular materials as a notable event of the last decade. Scientists have recently developed a theoretical approach to describe the motion of granular materials in a vibrating environment. This theory correctly describes the unexpected formation of stripe, square, and hexagon patterns on the surface of vibrated granular media and the formation of localized excitations called "oscillons." The theory also predicted how to control aspects of granular motion -- a prediction that was confirmed by experiment. The new theory brings the description and control of granular motion to a higher level of understanding and shows promise of substantial advances in basic granular science, which can lead to industrial applications that exploit the controlled motion of granular materials.

Vortex Matter -- A New Understanding of Magnetism in Superconductors. Magnetic fields in superconductors are carried by "vortices." Each vortex consists of a tube of magnetic field surrounded by a circulating flow of electrons that move without resistance. It is this free flow of electrons that gives superconducting materials their special property. Recently, it has been shown that the system of magnetic vortices can take many forms analogous to the solid, liquid, and gaseous forms of ordinary matter. The analogy between the behavior of vortices and ordinary matter is so strong that a new term has entered the scientific vocabulary -- vortex matter. Vortex matter melts from a crystalline to a liquid state in much the same way that ice melts to water. The properties of vortex matter can be controlled over a wide range. For example, the density of vortices can be varied by a factor of 10,000 simply by changing the applied magnetic field. This remarkable control enables the study of many types of phenomena in vortex matter whose analogies in ordinary matter are difficult or impossible to observe. Thus, the identification and characterization of the melting transition in vortex matter has significant implications for phase transitions in ordinary matter, for understanding the electromagnetic properties of superconductors, and for developing applications of superconductivity.

Chemical Sciences Subprogram

Landmark Experiment Challenges Combustion Models. Combustion is perhaps the oldest technology in human experience, yet its complexity limits predictions of combustion processes in devices ranging from simple laboratory burners to automobile engines. The challenge is characterizing the influence of chemistry and fluid dynamics on one another. A simple experiment recently has demonstrated a major error in current models for combustion processes. The experiment allows the interaction of chemistry and turbulence to be examined in quantitative detail for the first time. A planar flame sheet is deformed by a puff of air generated by a small loudspeaker. Spectroscopic techniques are used to determine the concentrations of reaction intermediates as the flame sheet deforms. Comparisons of these experiments with computational simulations showed that the widely accepted chemical reaction mechanism for simple methane combustion is in error, thus, requiring a fundamental change in our models for combustion.

Fishing for Radioactive Actinides with Molecular Hooks. The selection, separation, and removal of radioactive actinide ions from complex aqueous waste stream mixtures remain vexing technical issues. The development of new, improved separation approaches will result in significant cost savings for nuclear waste treatments as well as improve environmental safety and materials safeguard security. A new family of chelate agents or "chemical fish hooks" suitable for the reversible "catch and release" of trivalent actinide ions in highly acidic solutions has been designed, prepared, and characterized. The latest chelate derivatives show separation characteristics that are especially suited to practical, batch type waste treatments.

First Isolation of a Catalytic Oxidation Intermediate. Despite worldwide efforts over the last 15 years on catalytic olefin oxidation, little progress has been made in extrapolating from ethylene (the smallest olefin) to larger olefins such as propylene. The key question -- the molecular mechanism of ethylene epoxidation (which gives us anti-freeze and polyester fibers) -- remains unresolved. Now, a combined experimental and theoretical tour de force has yielded the first definitive isolation and spectroscopic characterization of a stable intermediate in the catalytic process -- an oxametallacycle. Calculations were employed to determine the structure for the oxametallacycle on silver and to predict the infrared spectrum and molecular motions for that structure. Conclusive identification was provided by the excellent agreement between the predicted infrared spectrum and the experimental electron energy loss spectrum.

Liquid Crystalline Organic Semiconductors Discovered. Liquid crystals change their optical properties as they transition between distinctive geometric states. Digital watch displays, for example, cycle between transparent and opaque forms. They, like other technologically important liquid crystals, are electrically insulating. Semiconducting crystals could have much broader application than insulating crystals, but large single crystals of these materials are difficult and expensive to produce. In a recent breakthrough, a family of liquid crystalline derivatives of perylene diimide was discovered that has semiconductor properties. The films of one compound self organize from a red, polycrystalline phase with randomly oriented crystallites into a black phase with highly ordered ribbon-like structure. The fluorescence intensity increases seven-fold during the transformation. This spontaneous change in photophysical properties makes this class of organic liquid crystals look very promising for future photoconversion applications.

Diode Lasers Detect Radiotoxic Isotopes. Solid-state diode lasers, similar to those used in compact disc players, have been used in a new approach to detect the toxic radioisotope strontium-90, which received attention because of high levels found in milk after atomic weapons tests and the Chernobyl reactor accident. Diode lasers excite and efficiently ionize the strontium atoms; the resulting ions are detected using a mass spectrometer. The high efficiency allows the detection of less than one femtogram (femto = 10⁻¹⁵, e.g., a single postage stamp compared to the area of Texas) of strontium 90. Furthermore, it is possible to selectively ionize the strontium 90 even in the presence of large excesses of the stable, naturally-occurring isotopes of strontium. Measurements can be performed in a few minutes as compared to the several weeks required previously for conventional radiochemical decay counting methods. Thus, this new approach should significantly improve the capabilities for near real-time monitoring of environmental restoration activities, nuclear weapons tests, reactor accidents, and the processing of nuclear fuels.

Photochemical Studies on the Light-Activated Drug Hypericin. The popular herbal remedy St. John's wort contains the compound hypericin, which upon exposure to light is toxic to tumors and HIV, the human AIDS virus. Now, the fundamental photochemistry of hypericin has been elucidated. A novel laser spectroscopic technique, fluorescence upconversion, was used to show definitively that the primary photochemical process is excited-state intramolecular proton or hydrogen transfer. Any incomplete proton or hydrogen atom transfers would acidify the aqueous solution immediately surrounding hypericin, which may be of importance in its toxicity to viruses. The study is yet another example of the role that the physical sciences play in providing fundamental information relevant to a wide variety of subject areas.

Engineering and Geosciences Subprogram

Remote Sensing of Fractures and Prediction of Failure in Rocks. Long before catastrophic fracturing and failure of a material, sound waves transmitted through the material show a dramatic frequency shift.

This shift has been documented before in fractured materials, but the observation of the shift before the formation of a continuous crack is a new discovery. Monitoring for the frequency shift can therefore be used to provide a warning of failure. The sound shifts to a lower frequency because the high-frequency sound (with shorter wavelengths) is preferentially absorbed or scattered. Because the frequency shift occurs prior to creation of a single fracture, there should be a network of oriented, disconnected features appearing prior to a crack that absorb or scatter the high-frequency sound in the same way as do observable cracks. Connected cracks in rocks provide pathways for water, oil, or pollutant flow. The growth of cracks can improve fluid flow or cause failure of well-bores, reservoirs, and tunnels or engineered structures; therefore, it is very important to understand how and when cracks form.

Energy Biosciences Subprogram

Building Doors into Cells. Before any molecule can enter a cell, it must first pass through the cell membrane—the thin, fat-containing film that covers all cells. The passage of most molecules through biological membranes is controlled by pores, defined openings made with specific proteins. The composition and structure of pore proteins can now be altered through genetic engineering. Changes in the size of the pore, the selectivity of the pore for letting different molecules pass through, and the pore's ability to open and close are three properties currently being studied by bioengineering new pore proteins. Successful attempts to engineer modified pore opening and closing properties have provided insight on how these processes can occur mechanistically as well as for developing new biotechnological applications. Among the potential products of this research are chemical triggers or molecular switches that can be used to create new sensors to detect harmful chemicals or viruses. Other potential applications are the development of small light switches and new drug delivery systems.

Selected FY 1997 Scientific Highlights/Accomplishments

The Advanced Photon Source (APS) Completes Its First Year of Operation. As the floor of the APS became crowded with experimental hutches, new results emerged that took advantage of the very high brightness of this new light source and that could not have been done elsewhere. While much of the work at the APS and the other BES synchrotron radiation light sources has been and will continue to be in the area of materials sciences and condensed matter physics, many studies are also being done in the areas of biological, plant, environmental, and geosciences. For example,

- A new structural determination and biochemical analysis of the human fragile histidine triad (FHIT) protein has been performed. The FHIT protein derives from a fragile site on human chromosome 3 that is commonly disrupted in association with cancers. The understanding of this tumor suppressor protein will focus on a diverse human HIT family member in search of their in vivo function throughout biology.
- The first experiments were conducted with a newly constructed beamline for geosciences/soil/environmental research. Molecular-scale observations (made possible by the high brightness of the APS) enable new understanding of local structural and chemical changes that govern the mechanisms of mineral-fluid interactions. For example, the molecular form or speciation of environmental contaminants, such as chromium, arsenic, lead, uranium or plutonium, determines their toxicity and bioavailability.
- Over 90% of the world's plants, including essentially all crops, make use of symbiotic associations with fungi. X-ray imaging studies performed on these systems using an x-ray microprobe have provided detailed information on the elemental distribution in plant roots and associated fungi. These images, with unprecedented spatial resolution, will be a key to understanding the symbiosis between the plant roots and fungi.

Materials Sciences Subprogram

Breakthrough in Processing of Aerogel Films. A breakthrough in the processing of ceramic aerogel films won a prestigious award of the American Chemical Society and was cited as an important discovery by the

Wall Street Journal. This breakthrough overcame the sixty year barrier to the large scale commercial utilization of these films. Aerogel films have a foam-like structure, exceptional lightness and transparency, and are ideal insulating materials for double-paned windows and other uses. When freshly formed from a liquid, the film can be easily torn until it has been hardened. Older processes required a toxic liquid and high pressure and temperature to dry the films. Employing a new understanding of film drying and chemical treatment of the surfaces of the pores in the film, a non-toxic, low-pressure and temperature process was developed to keep the film flexible and resilient as it formed.

Cool Sounds. Air conditioning from your favorite music? Not quite yet. However, sound, or acoustic energy, has now been used to make refrigerating and heating units. These devices, called thermoacoustic refrigerators, or thermoacoustic engines when operated in a heating mode, have no moving parts and use sound waves in air or helium to transfer heat. Operation of these devices has been based upon a standing acoustic wave in a closed system, limiting their usage. Now, a radically new concept has been devised in which the air or helium would flow slowly through the device during operation. This concept would allow for heating and cooling of buildings and for other industrial air conditioning applications with an economic advantage over current technology through the elimination of the bulky heat exchangers on building roofs. First results from a test system operating as a refrigerator using helium or air have confirmed the concept. Further developments of this concept are under way.

Slick and Sticky. Pencil-shaped organic molecules called "rod-coils," designed and synthesized to have half of the molecule rigid and the other half flexible, were discovered to exhibit unusual and important clustering mechanisms on several size scales. Aggregates of these molecules self-assemble into mushroom-shaped clusters with the rigid ends forming the stems and the flexible coils forming the caps. At the next level of organization, the mushroom clusters pack side by side into layered sheets to form, ultimately, a thick film. Because the building-block molecules are all oriented in the same direction, the film's properties mirror those of the individual molecules, resulting in a film whose bottom surface is sticky and top surface is slippery. Such a film has many potential applications, for example as an anti-ice coating on an airplane wing or an anti-blood-clot lining for artificial blood vessels. This new molecular organizational technique is being explored to make films with other properties by replacing the slippery and sticky groups capping the rodcoils with compounds that perform other functions, such as conducting electricity or changing their size in response to an electrical pulse.

Materials Failure in a Radiation Environment. The safe storage of nuclear materials and radioactive wastes is a major challenge for the post cold-war generation. The long term effects of radiation on the physical integrity of these materials and their containers is still poorly understood. Recent work using simultaneous electron microscopy and ion irradiation experiments shows that the impact of just a single high energy ion on the surface of a material has a much greater effect than previously realized and disrupts tens of thousands of atoms near the surface of the material. The impact causes local melting, displacement of many atoms beneath the surface, and the formation of surface craters and holes. This work should lead to a correct understanding of how materials are damaged by radiation and will help explain and predict the behavior of materials used for waste storage and other applications.

Powder Process Produces Cheaper Stronger Permanent Magnets. A collaborative team from two laboratories is a recipient of a prestigious R&D 100 Award for the processing of nanocrystalline composite powder for high-strength, permanent magnets. The permanent magnet industry is a very large global industry worth 3.2 billion dollars in 1995 and is predicted to reach 10 billion dollars by 2010. The high magnetic strength of the prize-winning neodymium-iron-boron 'super magnets' results from matching the crystallite size formed on cooling the alloy from the melt to the size of the magnetic domains. The previously used rapid cooling process that creates the fine-grained polycrystalline material is too expensive for many commercial magnet applications. It was discovered that adding titanium and carbon to the molten alloy allows a spray atomization process to create appropriately sized particles that can be consolidated into magnetic compacts.

New Process Forms Diamond-Like Boron Nitride Films. A process to grow diamond-like boron nitride films, the second hardest material known, has been discovered based on a new understanding of how hard nitride films are formed. Like diamond, films of boron nitride can be grown from hot gases and plasmas

without the use of high pressures. However, it was recently discovered that irradiation of boron nitride films with low-energy ion beams will produce films of boron nitride that contain the hard, diamond-like form rather than the soft graphite-like form. This new process to form ultra-hard boron nitride films could revolutionize the tool industry, because, unlike diamond, boron nitride does not react with iron or steel; therefore, boron nitride is an ideal material for cutting tools.

A Microscopic Understanding of Materials Joining Enables the Intelligent Processing of Materials.

Welding is a critical fabrication technology used extensively in a wide variety of industries such as energy, automotive, construction, aerospace, shipbuilding, and electronics. Weld failures are among the most common reason for unscheduled outages in power plants with the cost of replacement power often exceeding \$1,000,000 per day. Recent advances in materials joining science have improved our understanding of the welding process and welded materials. With the help of massively parallel computers, complex physical models that link both macro- and microscopic scale phenomena during the melting and solidification of a weld have been developed. Using such models it is now possible to visualize directly the solidified weld microstructure for a given set of processing conditions. The resulting knowledge has been transferred to industry thereby allowing the intelligent processing of defect-free, structurally sound and reliable welds.

Magnetic Refrigeration to Eliminate Harmful Freon. Conventional air conditioning of domestic and commercial buildings, and cooling in food processing and other industrial plants requires enormous quantities of electricity and uses huge amounts of environmentally harmful chlorofluorocarbons (CFCs). Magnetic refrigeration uses the magneto-caloric effect, the ability of a magnetic material to raise its temperature upon application of a magnetic field and to lower it upon removal of that field. For many years the alloys showing this effect operated only at impracticably low temperatures. New understanding of thermal and magnetic behavior uncovered a gadolinium-silicon-germanium alloy that cools efficiently near room temperature. Refrigerator devices based on magneto-caloric material could cut energy costs and eliminate ozone-depleting CFCs.

Chemical Sciences Subprogram

"Green" Separation Process for Hanford Wastes. The radioactive components in the Hanford waste tanks comprise a mere 1/100th of a percent of the millions of gallons of contaminated waste in storage. Thus, highly selective removal of the radioactive components could significantly reduce the volume of waste, which will require very costly processing and long-term storage. Fundamental studies of technetium extraction in the 1980s, followed by more recent investigations of the structural and thermodynamic aspects of the extraction of alkali metal salts with crown ethers has led to a new technetium extraction process. The crown ether binds sodium ions already present in the waste, and then extracts technetium as much as four orders of magnitude better than others ions in the waste, such as nitrate, which are present at much higher concentrations. The crown ether complex is readily decomposed by contact with water to release the extracted technetium thereby affording a convenient, safe, and economical stripping method. The crown ether is then recycled thus minimizing secondary waste production.

New Metallocene Catalysts Lead to Commercial Applications. The new family of metallocene polymerization catalysts, in which polymerization occurs principally at a single type of metal center with a well-defined coordination environment, are a substantial advance over the prior heterogeneous polymerization catalysts. Recent advances on two fronts -- strained early transition metals and non-coordinating counterions -- have resulted in new commercial applications by Dow Chemical and by Exxon Chemical. The remarkable stereospecificity features of these new catalysts have not only led to a variety of new, advanced polymer products over a wide range of densities, but they also provide the ability to "turn a microscope on" the underlying molecular mechanisms, thus leading to continually improved catalysts and products. The new polymers produced from these catalysts are found in wide-ranging applications from food wrapping to the plastic front end front bumper combinations on automobiles. The impact of these new products can be imagined from the Dow Insite process, which produces plastics with a market of about \$2,000,000,000 per year at Dow's Texas plant.

Joint Program Results in a New "Smart" Window. Windows with reduced transmission have been shown to be energy savers by reflecting some of the heat from solar radiation. However, such windows have fixed transmission that also reduces visible light. On a cloudy day a building or home equipped with such windows may not have adequate natural lighting. Research jointly supported by BES and the Department's Energy Efficiency program has led to the initial development of a self-powered "smart" window that can control its own transparency. Integration of two technologies, electrochromic windows and dye-sensitized solar cells, yields a smart window that darkens, reversibly, when exposed to sunlight.

Engineering and Geosciences Subprogram

Fast-Transport Predicted in Subsurface Fluids. Underground flow properties of fluids containing two or more components (oil(s)/water) are a major issue for environmental remediation. New experimental work documents how upward and downward flow of different fluids can be driven by differences in their density and their tendency to diffuse. Such transport occurs much more rapidly than has been predicted by earlier models. This new research developed innovative experimental methods to test the earlier predictions, and successfully measured and modeled the effects of multiphase flow in simple porous materials. This work is a significant step towards developing improved models to make better predictions for complex and highly variable natural subsurface environments.

Energy Biosciences Subprogram

New Sensor Provides Instant Litmus Test for Pathogens. A new class of colorimetric sensor materials has been invented that makes it possible to instantaneously and inexpensively detect a wide range of biological toxins and common disease-causing organisms. Building on earlier discoveries, researchers have developed a thin film consisting of receptor molecules attached to a film of linked diacetylene molecules. The film transmits blue light. The surface receptor molecules are designed to very selectively bind specific pathogens causing the film molecules to reorganize and the film to turn red. Pathogens thus far detected with good sensitivity include an influenza virus, cholera toxin, botulism toxin, and the toxin produced by the bacteria responsible for 200 deaths per year in the US alone, as noted by the recent contamination of fruit drinks and fast food hamburgers. Existing tests for all of these pathogens require at least a 24 hour culture. After further development, the sensors can be placed on plastic, paper, or glass and incorporated into inexpensive packaging and portable detection devices.

Silicon in Biology. Silicon is an element that is a principal component of glass, computer chips, coatings and numerous consumer products. There are only a few biological systems that metabolize this element. Silicon is metabolized by some simple animals, by algae to make the equivalent of glass houses, and by some higher plants (the rough feel of corn leaves comes from shards of silicates in the leaves). Recently a gene was identified that encodes a protein that is involved in binding and transporting silicon into a cell. This discovery will extend our understanding of how silicon is taken up and processed by biological systems which may lead to applications such as the mining of silicon from seawater and the manufacture of silicon-containing products.

Bioproduction of Natural Gas. The few microorganisms that possess the ability to produce methane (natural gas) have been studied for a number of years in the hope of using these organisms to produce a renewable energy source. Last year the genome of a methane-producing bacterium was sequenced which showed the uniqueness of these organisms. It is now thought that these bacteria are among the first life forms ever developed on earth. Recently, procedures have been developed which will permit the genes of methane-producing bacteria to be manipulated. This development will allow scientists to determine the nature and properties of these organisms and their unusual metabolism.

Controlling Natural Energy Resources through Plant Genetic Engineering. Cellulose is the most prevalent biological compound on earth. It is the principal component of all plants, wood, paper and cotton. When considered globally, cellulose constitutes an enormous supply of chemical energy, all of it renewable. Recently, several plants have been manipulated to make significantly less cellulose. This modification is important because it may now permit identification of the factors that control the synthesis and deposition of cellulose and related compounds. This development may permit the genetic engineering

of plants to produce either more cellulose, or plants that produce larger amounts of other chemicals such as liquid fuels and plastics.